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* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JUL 02	LMEDLINE coverage updated
NEWS	3	JUL 02	SCISEARCH enhanced with complete author names
NEWS	4	JUL 02	CHEMCATS accession numbers revised
NEWS	5	JUL 02	CA/Capplus enhanced with utility model patents from China
NEWS	6	JUL 16	Capplus enhanced with French and German abstracts
NEWS	7	JUL 18	CA/Capplus patent coverage enhanced
NEWS	8	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS	9	JUL 30	USGENE now available on STN
NEWS	10	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS	11	AUG 06	FSTA enhanced with new thesaurus edition
NEWS	12	AUG 13	CA/Capplus enhanced with additional kind codes for granted patents
NEWS	13	AUG 20	CA/Capplus enhanced with CAS indexing in pre-1907 records
NEWS	14	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS	15	AUG 27	USPATOLD now available on STN
NEWS	16	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS	17	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS	18	SEP 13	FORIS renamed to SOFIS
NEWS	19	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS	20	SEP 17	CA/Capplus enhanced with printed CA page images from 1967-1998
NEWS	21	SEP 17	Capplus coverage extended to include traditional medicine patents
NEWS	22	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	23	OCT 02	CA/Capplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS	24	OCT 19	BEILSTEIN updated with new compounds
NEWS EXPRESS	19	SEPTEMBER 2007:	CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS LOGIN			Welcome Banner and News Items
NEWS IPC8			For general information regarding STN implementation of IPC 8

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 06:20:28 ON 13 NOV 2007

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 06:20:45 ON 13 NOV 2007

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DICTIONARY FILE UPDATES: 12 NOV 2007 HIGHEST RN 953132-99-5

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

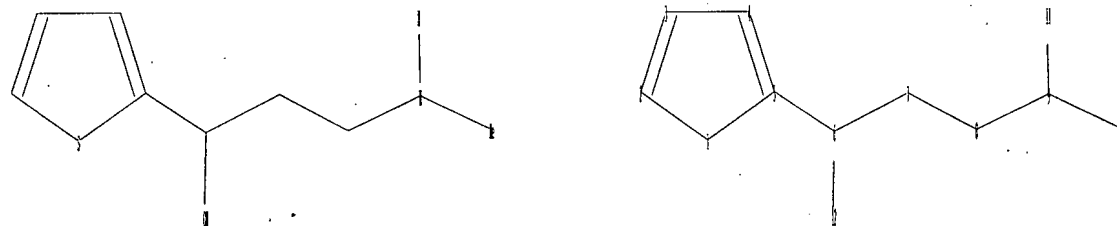
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<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10522888\Struc 1.str



chain nodes :

6 7 8 9 10 11 12

ring nodes :

1 2 3 4 5

chain bonds :

5-6 6-7 6-12 7-8 8-9 9-10 9-11

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

10522888.trn

Page 3

1-2 1-5 2-3 3-4 4-5 6-12 8-9
exact bonds :
5-6 6-7 7-8 9-10 9-11

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS

L1 STRUCTURE UPLOADED

=> l1 exa full

FULL SEARCH INITIATED 06:20:56 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 78 TO ITERATE

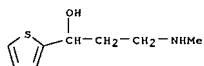
100.0% PROCESSED 78 ITERATIONS
SEARCH TIME: 00.00.01

5 ANSWERS

L2 5 SEA EXA FUL L1

=> d scan

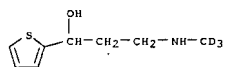
L2 1 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-
MF C8 H13 N O S
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

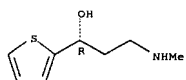
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L2 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 2-Thiophenemethanol, α-[2-(methyl-d3-amino)ethyl]-
MF C8 H10 D3 N O S
CI COM



L2 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)-
MF C8 H13 N O S
CI COM

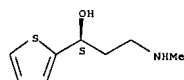
Absolute stereochemistry, Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)-
MF C8 H13 N O S
CI COM

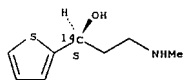
Absolute stereochemistry, Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 2-Thiophenemethanol- α -14C, α -[2-(methylamino)ethyl]-, (S)-
(9CI)
MF C8 H13 N O S

Absolute stereochemistry.



ALL ANSWERS HAVE BEEN SCANNED

Page 6

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
58.25	58.46

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 06:21:19 ON 13 NOV 2007
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FILE COVERS 1907 - 13 Nov 2007 VOL 147 ISS 21
FILE LAST UPDATED: 12 Nov 2007 (20071112/ED)

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=> 12

L3 52 L2

=> 13 and hydrolase

23634 HYDROLASE

L4 1 L3 AND HYDROLASE

=> d scan

10522888.trn

L4 1 ANSWERS CAPLUS COPYRIGHT 2007 ACS on STN
 IC ICM C07D333-20
 ICS C07B057-00
 CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 7
 TI Preparation of enantiomerically pure (S)-3-methylamino-1-(thien-2-yl)propan-1-ol from racemic 3-hydroxy-3-(thien-2-yl)propionitrile via kinetic resolution with an acylating agent and a lipase followed by treatment with methylamine and hydrogen in the presence of a catalyst.
 ST hydroxythienylpropionitrile chiral reductive amination; methylaminothienylpropanol enantiomerically pure prep
 IT Resolution (separation)
 (kinetic; preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)
 IT Burkholderia
 Burkholderia cepacia
 Burkholderia glumae
 Burkholderia plantarii
 Chryseomonas luteola
 Pseudomonas
 Pseudomonas aeruginosa
 Pseudomonas fluorescens
 Pseudomonas fragi
 Pseudomonas vulgaris
 Pseudomonas wisconsinensis
 (lipases; preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)
 IT Amination catalysts
 (reductive; palladium, nickel; preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)
 via kinetic resolution followed by catalytic reductive amination with methylamine)
 IT Amination
 (reductive; preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)
 IT 7440-02-0, Raney nickel, uses
 RL: CAT (Catalyst use); USES (Uses)
 (catalysts; preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)
 IT 9001-62-1, Lipase
 RL: CAT (Catalyst use); USES (Uses)
 (from Pseudomonas DSM 8246; preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)

L4 1 ANSWERS CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 kinetic resoln. followed by catalytic reductive amination with methylamine)
 IT 591727-36-5P
 RL: BPN (Biosynthetic preparation); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)
 IT 7440-05-3, Palladium, uses
 RL: CAT (Catalyst use); USES (Uses)
 (preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)
 IT 116539-55-0P, (S)-3-Methylamino-1-(thien-2-yl)propan-1-ol
 RL: IMP (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)
 IT 67-56-1, Methanol, uses 1634-04-4, Methyl tert-butyl ether
 RL: NUU (Other use, unclassified); USES (Uses)
 (preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)
 IT 74-89-3, Methylamine, reactions 75-05-8, Acetonitrile, reactions 98-03-3, Thiophene-2-carboxaldehyde 105-38-4, Vinyl propionate 108-30-5, Succinic anhydride, reactions 3050-69-9, Vinyl hexanoate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)
 IT 235085-83-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)

ALL ANSWERS HAVE BEEN SCANNED

Page 8

=> d ibib abs hitstr

10522888.trn

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:120843 CAPLUS

DOCUMENT NUMBER: 140:181317

TITLE: Preparation of enantiomerically pure (S)-3-methylamino-1-(thien-2-yl)propan-1-ol from racemic 3-hydroxy-3-(thien-2-yl)propionitrile via kinetic resolution with an acylating agent and a lipase followed by treatment with methylamine and hydrogen in the presence of a catalyst.

INVENTOR(S): Stuermer, Rainer

PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 31 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004013123	A1	20040212	WO 2003-EP8492	20030731
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
DE 10235206	A1	20040219	DE 2002-10235206	20020801
CA 2493451	A1	20040212	CA 2003-2493451	20030731
AU 2003251677	A1	20040223	AU 2003-251677	20030731
EP 1527065	A1	20050504	EP 2003-766383	20030731
EP 1527065	B1	20061122		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
CN 1671687	A	20050921	CN 2003-818510	20030731
JP 2006507234	T	20060302	JP 2004-525403	20030731
AT 346061	T	20061215	AT 2003-766383	20030731
ES 2278203	T3	20070801	ES 2003-3766383	20030731
US 2005245749	A1	20051103	US 2005-522888	20050624
PRIORITY APPLM. INFO.:			DE 2002-10235206	A 20020801
			WO 2003-EP8492	W 20030731

OTHER SOURCE(S): CASREACT 140:181317

AB A process for the preparation of enantiomerically pure (S)-3-methylamino-1-(thien-2-yl)propan-1-ol (I) comprises treatment of a mixture of (R)- and (S)-3-hydroxy-3-(thien-2-yl)propionitrile with an acylating agent in the presence of a hydrolase to give a mixture of unacylated (S)-3-hydroxy-3-(thien-2-yl)propionitrile and acylated (R)-nitrile and treatment of the former with hydrogen and methylamine in the presence of

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

catalyst. Thus, 3-hydroxy-3-(thien-2-yl)propionitrile (prepn. given) was shaken with lipase from Pseudomonas DSM 8246 and vinyl hexanoate in Me tert-Bu ether for 6 h at room temp. to give after flash chromatog. 48% (S)-3-hydroxy-3-(thien-2-yl)propionitrile in 99.4% enantiomeric excess.

The latter was autoclaved with MeNH₂ in MeOH over Raney Ni under 50 bar H₂ at 65° for 24 h to give 79% I.

IT 116539-55-0P, (S)-3-Methylamino-1-(thien-2-yl)propan-1-ol

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP

(Preparation)

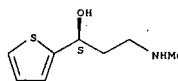
(preparation of enantiomerically pure methylaminothiethylpropanol from racemic hydroxythienylpropionitrile via kinetic resolution followed by catalytic reductive amination with methylamine)

RN 116539-55-0 CAPLUS

CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- ICA

INDEX NAME)

Absolute stereochemistry. Rotation (-).



=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

8.22

66.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-0.78

-0.78

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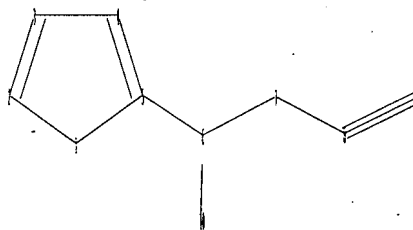
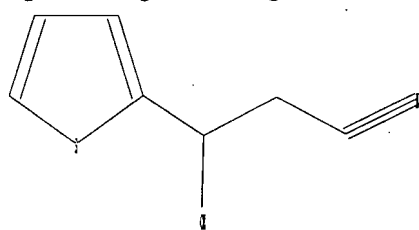
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<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10522888\Struc 2.str



chain nodes :

6 7 8 9 10

ring nodes :

1 2 3 4 5

chain bonds :

5-6 6-7 6-10 7-8 8-9

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 6-10 8-9

exact bonds :

Page 11

5-6 6-7 7-8

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS

L5 STRUCTURE UPLOADED

=> l5 exa full

FULL SEARCH INITIATED 06:23:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 17 TO ITERATE

100.0% PROCESSED 17 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

L6 3 SEA EXA FUL L5

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	58.25	124.93

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.78

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DICTIONARY FILE UPDATES: 12 NOV 2007 HIGHEST RN 953132-99-5

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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conducting SmartSELECT searches.

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predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> l2 and l6

L7 0 L2 AND L6

10522888.trn

=> 16

SAMPLE SEARCH INITIATED 06:23:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 40 TO ITERATE

100.0% PROCESSED 40 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 421 TO 1179
PROJECTED ANSWERS: 2 TO 124

L8 2 SEA SSS SAM L5

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.45	125.38

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.78

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FILE COVERS 1907 - 13 Nov 2007 VOL 147 ISS 21
FILE LAST UPDATED: 12 Nov 2007 (20071112/ED)

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=> 12 and 16

52 L2
9 L6
L9 4 L2 AND L6

=> d ibib abs hitstr 1-4

L9 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2004:286808 CAPLUS

DOCUMENT NUMBER:

140:302436

TITLE:

Process for the production of 3-heteroaryl-3-hydroxy-propionic acid derivatives by enantioselective microbial reduction

INVENTOR(S):

Berendes, Frank; Eckert, Markus; Brinkmann, Nils; Dreisbach, Claus; Meissner, Ruth; Koch, Rainhard

PATENT ASSIGNEE(S):

Bayer Chemicals A.-G., Germany

SOURCE:

Eur. Pat. Appl., 16 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1405917	A2	20040407	EP 2003-20847	20030913
EP 1405917	A3	20050112		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
DE 10244811	A1	20040408	DE 2002-10244811	20020926
IN 2003MU00922	A	20050715	IN 2003-MU922	20030908
US 2004181056	A1	20040916	US 2003-669424	20030924
JP 2004113245	A	20040415	JP 2003-335690	20030926
CN 1497048	A	20040519	CN 2003-160307	20030926
US 2006264641	A1	20061123	US 2006-436347	20060518
PRIORITY APPLN. INFO.:				
DE 2002-10244811 A 20020926				
US 2003-669424 A3 20030924				

OTHER SOURCE(S):

MARPAT 140:302436

AB A process for the production of 3-heteroaryl-3-hydroxy-propionic acid derivs.

by enantioselective microbial reduction is provided. Thus, *Saccharomyces cerevisiae* was used to reduce methyl-3-oxo-3-(2-thiophenyl)propanoic acid to methyl-(3S)-hydroxy-3-(2-thiophenyl)propanoic acid with a yield of 75% and an enantiomeric excess >97%. The reaction product then served as a reactant in the chemical synthesis of

(1S)-3-(methylamino)-1-(2-thienyl)-1-propanol.

IT 116539-55-0P 116539-57-2P, (1R)-3-(Methylamino)-1-(2-thienyl)-1-propanol 591727-36-5P, (S)-3-Hydroxy-3-(2-thienyl)propanenitrile

RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)

(process for production of 3-heteroaryl-3-hydroxy-propionic acid

derivs. by

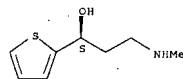
enantioselective microbial reduction)

RN 116539-55-0 CAPLUS

CN 2-Thiophenemethanol, α -[2-(methylamino)ethyl]-, (aS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

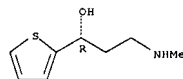
L9 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 116539-57-2 CAPLUS

CN 2-Thiophenemethanol, α -[2-(methylamino)ethyl]-, (aR)- (CA INDEX NAME)

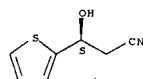
Absolute stereochemistry. Rotation (+).



RN 591727-36-5 CAPLUS

CN 2-Thiophenepropanenitrile, β -hydroxy-, (HS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L9 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2004:198151 CAPLUS

DOCUMENT NUMBER:

140:253344

TITLE:

Preparation of (3R) - or (3S)-3-oxy-3-(2-thiophen)propylamines and related compounds via an enantioselective Reformatskii reaction

INVENTOR(S):

Sorgert, Klaus; Stratmann, Oliver; Petersen, Hermann; Stohrer, Juergen

PATENT ASSIGNEE(S):

Consortium fuer Elektrochemische Industrie G.m.b.H., Germany

SOURCE:

Ger. Offen., 29 pp.

CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10237272	A1	20040311	DE 2002-10237272	20020814
PRIORITY APPLN. INFO.:				
DE 2002-10237272 20020814				

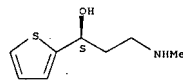
OTHER SOURCE(S):

MARPAT 140:253344

GI

L9 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

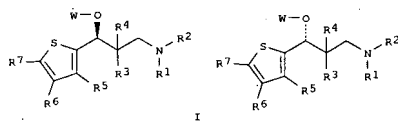
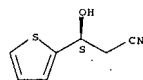
Absolute stereochemistry. Rotation (-).



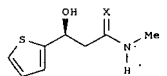
RN 591727-36-5 CAPLUS

CN 2-Thiophenepropanenitrile, β -hydroxy-, (HS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



II



III

AB Title compds. I and II [R1, R2 = H, halo-alkyl, CN-alkyl; R3, R4, R5, R6, R7 = H, halo, halo-alkyl; W = H, alkyl, acyl, etc.] were prepared via a sparteine mediated enantioselective Reformatskii reaction. For example, LAH reaction of amide II (X = O), e.g., prepared from 2-thiophenecarboxaldehyde in 2-steps, afforded propylamine in 90% yield and 89% ee (HPLC).

IT 116539-55-0P, N-Methyl-(S)-(-)-3-Hydroxy-3-(2-thiophen)propylamine 591727-36-5P, (S)-(-)-3-Hydroxy-3-(2-thiophen)propane nitrile

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of (3S)-3-oxy-3-(2-thiophen)propylamines and related compds.

via an enantioselective Reformatskii reaction)

RN 116539-55-0 CAPLUS

CN 2-Thiophenemethanol, α -[2-(methylamino)ethyl]-, (aS)- (CA INDEX NAME)

10522888.trn

L9 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:120843 CAPLUS

DOCUMENT NUMBER: 140:181317

TITLE: Preparation of enantiomerically pure (S)-3-methylamino-1-(thien-2-yl)propan-1-ol from racemic 3-hydroxy-3-(thien-2-yl)propanenitrile via kinetic resolution with an acylating agent and a lipase followed by treatment with methylamine and hydrogen in the presence of a catalyst.

INVENTOR(S): Stuermer, Rainer

PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 31 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

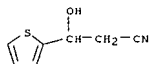
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WO 2004013123	A1	20040212	WO 2003-EP8492	20030731
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10235206	A1	20040219	DE 2002-10235206	20020801
CA 2493451	A1	20040212	CA 2003-2493451	20030731
AU 2003251677	A1	20040223	AU 2003-251677	20030731
EP 1527065	A1	20050504	EP 2003-766383	20030731
EP 1527065	B1	20061122		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1671687	A	20050921	CN 2003-618510	20030731
JP 2006507234	T	20060302	JF 2004-525403	20030731
AT 346061	T	20061219	AT 2003-766383	20030731
ES 2278203	T3	20070801	ES 2003-3766383	20030731
US 2005245749	A1	20051103	US 2005-522888	20050624
			DE 2002-10235206	A 20020801
			WO 2003-EP8492	W 20030731

OTHER SOURCE(S):

CASREACT 140:181317

AB A process for the preparation of enantiomerically pure (S)-3-methylamino-1-(thien-2-yl)propan-1-ol (I) comprises treatment of a mixture of (R)- and (S)-3-hydroxy-3-(thien-2-yl)propanenitrile with an acylating agent in the presence of a hydrolase to give a mixture of unacylated (S)-3-hydroxy-3-(thien-2-yl)propanenitrile and acylated (R)-nitrile and treatment of the former with hydrogen and methylamine in the presence of a catalyst. Thus,

L9 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L9 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

3-hydroxy-3-(thien-2-yl)propanenitrile (prepn. given) was shaken with lipase from *Pseudomonas* DSM 8246 and vinyl hexanoate in Me tert-Bu ether for 6 h at room temp. to give after flash chromatog. 48% (S)-3-hydroxy-3-(thien-2-yl)propanenitrile in 99.4% enantiomeric excess. The latter was autoclaved with MeNH₂ in MeOH over Raney Ni under 50 bar H₂ at 65° for 24 h to give 75% I.

IT 591727-36-5P

RL: BPN (Biosynthetic preparation); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant)

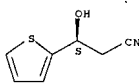
or

reagent) [preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropanenitrile via kinetic resolution followed by catalytic reductive amination with methylamine]

RN 591727-36-5 CAPLUS

CN 2-Thiophenepropanenitrile, β-hydroxy-, (1S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 116539-55-0P, (S)-3-Methylamino-1-(thien-2-yl)propan-1-ol

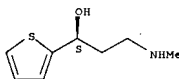
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

[preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropanenitrile via kinetic resolution followed by catalytic reductive amination with methylamine]

RN 116539-55-0 CAPLUS

CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 235085-83-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

[preparation of enantiomerically pure methylaminothienylpropanol from racemic hydroxythienylpropanenitrile via kinetic resolution followed by catalytic reductive amination with methylamine]

RN 235085-83-3 CAPLUS

CN 2-Thiophenepropanenitrile, β-hydroxy-, (CA INDEX NAME)

L9 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:405867 CAPLUS

DOCUMENT NUMBER: 139:245838

TITLE: Chemoenzymatic synthesis of duloxetine and its enantiomer: lipase-catalyzed resolution of 3-hydroxy-3-(2-thienyl)propanenitrile

AUTHOR(S): Kamal, Ahmed; Khanna, G. B. Ramesh; Ramu, R.; Krishnaji, T.

CORPORATE SOURCE: Division of Organic Chemistry, Biotransformation Laboratory, Indian Institute of Chemical Technology, Hyderabad, 500 007, India

SOURCE: Tetrahedron Letters (2003), 44(25), 4783-4787

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:245838

AB An efficient and facile chemoenzymatic synthesis of duloxetine by lipase-mediated resolution of 3-hydroxy-3-(2-thienyl)propanenitrile has been achieved. This process also describes an enantioconvergent synthesis of duloxetine via a Mitsunobu reaction.

IT 116539-55-0P 116539-57-2P 524047-48-1P

591727-36-5P

RL: BPN (Biosynthetic preparation); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant)

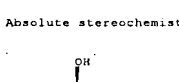
or

reagent) [chemoenzymic synthesis of duloxetine and its enantiomers via lipase-catalyzed resolution of hydroxy(thienyl)propanenitrile and its use in enantioconvergent synthesis of duloxetine via Mitsunobu reaction]

RN 116539-55-0 CAPLUS

CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

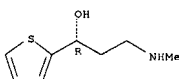
Absolute stereochemistry. Rotation (+).



RN 116539-57-2 CAPLUS

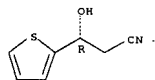
CN 2-Thiophenemethanol, α-[2-(methylamino)ethyl]-, (αR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



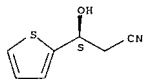
L9 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 RN 524047-48-1 CAPLUS
 CN 2-Thiophenepropanenitrile, β -hydroxy-, (1R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

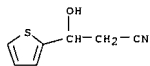


RN 591727-36-5 CAPLUS
 CN 2-Thiophenepropanenitrile, β -hydroxy-, (1S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 235085-83-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (chemoenzymic synthesis of duloxetine and its enantiomers via
 lipase-catalyzed resolution of hydroxy(thienyl)propanenitrile and its
 use in enantioconvergent synthesis of duloxetine via Mitsunobu reaction)
 RN 235085-83-3 CAPLUS
 CN 2-Thiophenepropanenitrile, β -hydroxy- (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR
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 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

Page 16

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COST IN U.S. DOLLARS

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SESSION

FULL ESTIMATED COST

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

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SESSION WILL BE HELD FOR 120 MINUTES

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